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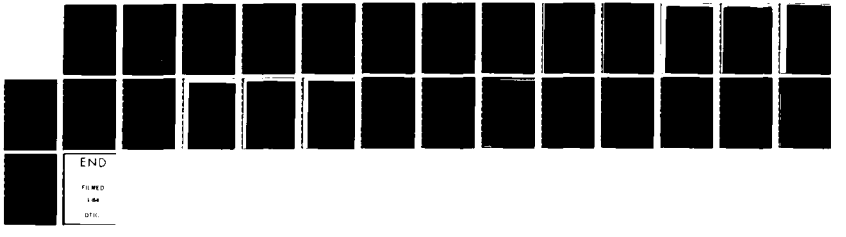

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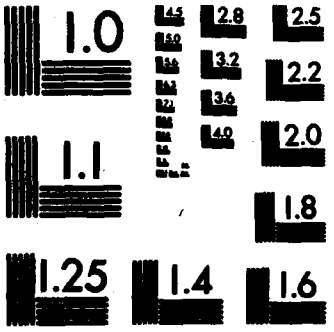

HIGH FIELD TRANSPORT OF FREE CARRIERS AT THE Si-SiO_2 INTERFACE

PROGRESS REPORT NO. 6
(FINAL REPORT)

K. HESS

OCTOBER 1983

U. S. ARMY RESEARCH OFFICE

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COORDINATED SCIENCE LABORATORY
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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Investigations of interface transport, ballistic transport and generally speaking high field transport in silicon and III-V compounds are reported.

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During the period of this contract 20 manuscripts (abstracts and reprints attached) were published or accepted for publication. Six manuscripts have been published or submitted for publication in the last period (January 1983 - September 1983) of this contract. Since the manuscripts are attached and the contract will be continued, only a short description of the major scientific progress is given here.

1. Ballistic Transport:

We have performed Monte Carlo simulations of high energy transient electronic transport for GaAs, InAs and InP including the effects of contacts and a realistic bandstructure. We found that ballistic transport and high drift velocities are possible only over distances smaller than 1500 Å. Our results are currently used by many groups to design high speed field effect and heterojunction bipolar devices.

2. Emission of Hot Electrons from Silicon into Silicon Dioxide

Our model calculations of this effect have shown that the emission takes place because of collision broadening effects due to the electron-phonon interaction. This means that the effect cannot be "scaled away" and will be important also for voltages much below 3V (the band edge discontinuity). Our findings have been confirmed experimentally by Muller and his group at Berkeley and will be important for the design of submicron MOS transistors.

3. Hot Electron Shockley Equations

We have derived a set of equations which generalize Shockleys Equations and include in a straightforward fashion hot electron effects (also diffusion).

4. Superlattices

We have developed a theory of superlattice bandstructure and found (Report #4) that by using two indirect semiconductor materials and zone folding it properly a direct superlattice material can be created. This indirect-direct transition is now investigated by several groups in the U.S.A.

A review on superlattice transport including some novel real space transfer application has also been written.

5. Deformation Potentials

We have developed a theory of deformation potential scattering in superlattices.

6. Random Superlattices

A theory of random superlattices has been developed together with J. D. Dow.

7. Scientific Personnel

K. Hess	Principal Investigator
J. P. Leburton	Visiting Assistant Professor
K. K. Mon	Post Doctoral Research Associate
Kent Byerly	Masters Degree Student, MS completed 1982
John Grieger	Masters Degree Student
Choon Lee	Masters Degree Student, MS completed 1983
J. Y. Tang	Ph.D. Degree Student, Ph.D. completed 1982
T. Wang	Ph.D. Degree Student

8. List of Publications:

J. Y. Tang, H. Shichijo, K. Hess and G. J. Iafrate, "Band-Structure Dependent Impact Ionization in Silicon and Gallium Arsenide," Journal De Physique pp. C7-63--C7-69 (1981).

K. K. Mon, K. Hess and J. D. Dow, "Deformation potentials of superlattices and interfaces," J. Vac. Sci. Technol., 19(3) pp. 564-566 (1981).

K. Hess and J. D. Dow, "Deformation Potentials of Bulk Semiconductors," Solid State Communications. Vol. 40, pp. 371-373 (1981).

John D. Dow, Shang Yuan Ren and Karl Hess, "Random superstructures," Physical Review B. Vol. 25, No. 8 (1982).

W. T. Jones, K. Hess and G. J. Iafrate, "Hot Electron Diffusion in Fine Line Semiconductor Devices," Solid-State Electronics, Vol. 25, No. 10, pp. 1017-1021 (1982).

Jeffrey Yuh-Fong Tang and Karl Hess, "Investigation of Transient Electronic Transport in GaAs Following High Energy Injection, IEEE Transactions on Electron Devices, Vol. ED-29, No. 12, pp. 1906-1911 (1982).

K. K. Mon, "Electronic Band Structure of (001) GaAs-AlAs Superlattices," Solid State Comm. 41, 699 (1982).

K. K. Mon, "Electronic Band Structure of a Model AlP-GaP Superlattice: Indirect to Direct Transition," unpublished.

J. P. Leburton and K. Hess, "High Energy Diffusion Equation for Polar Semiconductors," Physica 117B & 118B, pp. 211-213 (1983).

J. P. Leburton and K. Hess, "Energy Diffusion Equation for an Electron Gas Interacting with Polar Optical Phonons," Phys. Rev. B 26, 5623 (1982).

J. P. Leburton, J. Tang and K. Hess, "Energy Diffusion Equation for an Electron Gas Interacting with Polar Optical Phonons: Non-Parabolic Case," Solid State Communications, Vol. 45, No. 6, pp. 517-519 (1983).

Jeffrey Yuh-Fong Tang and Karl Hess, "Investigation of Transient Electronic Transport in GaAs Following High Energy Injection," IEEE Transactions on Electron Devices, Vol. ED-29, No. 12 (1982).

T. Wang, J. P. Leburton and Karl Hess, "A Jet-Stream Solution for the Current in Planar-Doped-Barrier Devices," presented at the Workshop on The Physics of Submicron Structures, University of Illinois, Urbana, IL, June 1982. Proceedings to be published.

G. J. Iafrate, R. J. Malik, J. Y. Tang and K. Hess, "Transient Transport and Transferred Electron Behavior in Gallium Arsenide Under the Condition of High-Energy Electron Injection," Solid State Communications 45, 255 (1983).

8. List of Publications (Continued)

K. Hess and G. J. Iafrate, "Hot Electrons in Semiconductor Heterostructures and Superlattices," Book Chapter, to be published by Springer.

K. Brennan, K. Hess, J. Y. Tang and G. J. Iafrate, "Transient Electronic Transport in InP Under the Condition of High-Energy Electron Injection," to be published in Trans. of IEEE on ED.

K. Brennan, K. Hess and G. J. Iafrate, "Monte Carlo Simulation of n-n+ Contact Behavior," to be published in IEEE-ED Letters.

K. Brennan and K. Hess, "High Field Transport in GaAs, InP, and InAs," to be published in Solid State Electronics.

J. Y. Tang and Karl Hess, "Theory of hot electron emission from silicon into silicon dioxide," J. Appl. Phys. 54(9), pp. 5145-5151 (1983).

K. Brennan and Karl Hess, "Transient Electronic Transport in Staircase Heterostructures," to be published in IEEE on ED Letters.

9. Ph.D. and Masters Theses:

Kent Byerly, "Effects of Oxygen Impurities in N-Type Silicon Conducting Layers," Masters Thesis, 1982.

Choon Lee, "The Electron Transport Properties in Layered Polar-Semiconductor Heterostructures," Masters Thesis, 1983.

Jeffrey Tang, "Theoretical Studies of High Field, High Energy Transport in Gallium Arsenide, Silicon and Heterostructures," Ph.D. Thesis, 1982.

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BAND-STRUCTURE DEPENDENT IMPACT IONIZATION IN SILICON AND GALLIUM ARSENIDE

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Résumé. - Nous avons développé une simulation par la méthode de Monte Carlo pour du silicium et de l'AsGa en incluant une structure de bande réaliste. Les taux d'ionisation par impact et les vitesses de dérive en régime continu sous forts champs électriques (>100 kV/cm) ont été calculés à différentes températures.

Abstract. - We have performed a Monte Carlo simulation for GaAs and Si with the realistic band structure included. Steady state impact ionization rates and drift velocities under high electric fields (> 100 kV/cm) were calculated at various temperatures.

1. Introduction. - Impact ionization is an essential mechanism in the operation of semiconductor devices such as avalanche photo-diodes or transit time devices. The dependence of impact ionization on the crystallographic orientation has attracted substantial interest because of its relevance to noise and other phenomena in these devices. This dependence, however, is not shown by any of the theories as given by Wolff [1], Shockley [2], and Baraff [3], since none of them include a realistic band structure.

We have developed a complete theory for impact ionization and generally high field transport in semiconductors by combining a Monte Carlo simulation with the realistic band structure calculated by the empirical pseudopotential method. We do take into account scattering by all possible phonon types, the change in the density of states high in the band, the exact velocity $\vec{v} = \frac{1}{\hbar} \nabla_k E(\vec{k})$ (no effective mass approximation), the collision broadening of the electronic states, and the temperature effect.

Details of the model and the results for GaAs at 300 K can be found in two of our previous papers [4,5]. In the case of Si, the first two conduction bands were included. Besides the X - X scattering we also include the X - L scattering in Si. In Section 2, we describe briefly our model and point out its differences from the commonly used model. The effects of the inclusions of the second band and the transition from X - L in Si are discussed in Section 4.

2. Theoretical Model. - The model for Monte Carlo simulation has two main ingredients: (i) the band structure and (ii) the scattering rate. We describe briefly in the following the different features that have been included in our model and the advantages it has over other models.

Deformation potentials of superlattices and interfaces

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(Received 23 February 1981; accepted 20 April 1981)

We present a theory of deformation potential electron–phonon scattering in the bulk, in superlattices, and at interfaces of semiconductors. Expressions for the acoustical deformation potential constants are obtained in closed form for bulk semiconductors and for a monolayer superlattice. Deformation potential constants are evaluated numerically for superlattices of various thicknesses. The results are in good agreement with available experiments and provide a detailed understanding of deformation potential scattering.

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One of the dominant scattering mechanisms of carriers in semiconductors involves long wavelength acoustical phonons. It was first pointed out by Bardeen and Shockley[1] that such interactions can be described by a deformation potential. The basic assumption is that the local lattice deformation produced by the phonons is equivalent to a homogeneous deformation of the crystals. The strength of this coupling, the deformation potential constant $[Z_n(\mathbf{k})]$ is then determined by the shifts in the (nth) energy band (at momentum $\mathbf{k}$) per unit of dilation ($\xi = \delta V/V$) produced by the acoustical waves,

$$Z_n(\mathbf{k}) = \frac{dE_n(\mathbf{k})}{d\xi}. \tag{1}$$

An understanding of deformation potential scattering is of fundamental importance for transport, optical, and other properties of bulk[2] semiconductors and superlattices. Despite advances[3] in electronic band structure calculations, there have been only a few calculations[4] of the deformation potential constants for a few selected bulk semiconductors and none in superlattices. The main difficulty is that the required absolute shift of the band edge is beyond most empirical band structure calculations where the relative band edges are fitted to agree with experimental observations. (See Kleinman, Ref. 4.) As a consequence, the deformation potential constants for the bulk are usually deduced from transport and optical measurements with various fitting schemes, often resulting in a range of experimental estimates.[5]

In this paper we summarize a theory for the deformation potential scattering by long wavelength acoustical phonons in bulk semiconductors[6]; and we extend the theory to superlattices and interfaces. We show that the absolute shift of the band edge can be obtained using an equilibrium sum rule. Expressions for the deformation potential constants are obtained in closed form for bulk semiconductors and the results are in very good agreement with experimental results. The theory is applied to semiconductor superlattices and closed form expressions for the deformation potential constants are given for monolayer superlattices. Results for lattice-matched AlAs/GaAs superlattices of various thickness are obtained numerically. To our knowledge this is the first calculation of deformation potential constants for interfaces and superlattices using realistic models of band structure. We show that for most practical cases the differences between superlattice and bulk deformation potential constants are small. The differences that do occur include a new "edge" scattering mechanism and are caused by band-edge discontinuities.

The electronic energy bands of a system of ions and electrons can be written as,

$$E_n(\mathbf{k}) = E_n{}^{BS}(\mathbf{k}) + E^o, \tag{2}$$

where E^o is related to the ion–ion self-energy and is usually chosen such that the zero of $E_n{}^{BS}(\mathbf{k})$ is at the maximum of the valence band. E_o contains contributions involving ions and electrons (see Kleinman, Ref. 5). It is density dependent and is very difficult to evaluate in general. Under dilation or changes in the lattice constants, a shift of the energy bands is produced,

$$\delta E_n(\mathbf{k}) = \delta E_n{}^{BS}(\mathbf{k}) + \delta E^o. \tag{3}$$

Although E^o is difficult to calculate, small changes in E^o can be easily approximated by an extension of techniques used by Chadi[7] in his ground state calculations involving total-energy minimization of surface atomic structures. One considers a sum over the occupied single particle states,

$$E_{tot} = \sum_{n,\mathbf{k}} E_n{}^{BS}(\mathbf{k}) + N_{tot}E_o, \tag{4}$$

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DEFORMATION POTENTIALS OF BULK SEMICONDUCTORS

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(*Received* 12 *May* 1981 *by J. Tauc*)

A theory of deformation potential electron–phonon scattering coefficients is presented for elemental and compound semiconductors. Expressions for the acoustical deformation potential constants at symmetry points are obtained in closed form for direct-gap bulk semiconductors. The deformation potential vs k is predicted for GaAs.

IN THIS PAPER we present a simple but successful theory of dilational deformation potentials for semiconductors, obtaining analytic expressions for bulk deformation potential constants in terms of empirical tight-binding energy band parameters.

The idea of a deformation potential was first enunciated by Bardeen and Schockley [1], who proposed that long-wavelength acoustic phonons be simulated by homogeneous lattice deformations, permitting one to calculate the electron–phonon scattering matrix elements or deformation potential constants $Z_n(\mathbf{k})$ by expanding the band structure to first order in the change of lattice constant da_L:

$$E_n(\mathbf{k}, a_L + da_L) = E_n(\mathbf{k}, a_L) + Z_n(\mathbf{k})(3da_L/a_L).$$

Thus the deformation potential constant $Z_n(\mathbf{k})$ is proportional to the derivative of the energy band with respect to the lattice constant a_L. (Here, for clarity of presentation, we have avoided the tensor character of $Z_n(\mathbf{k})$ by considering only purely dilational strains: $\xi \equiv dV/V = 3da_L/a_L$; a complete discussion of the tensor character will be published separately.)

As shown by Kleinman [2], the one main difficulty in computing deformation potential constants arises because of a difficult-to-evaluate many-body self-energy contribution [3]. We circumvent the direct calculation of the many-body term by using a sum rule [3, 4] to express it in terms of easily calculable one-body quantities.

To illustrate this point, we consider the simple example of the following one electron Hamiltonian:

$$H = p_i^2/2m + V(\mathbf{r}_i; \mathbf{R}) + S(\mathbf{r}_i; \mathbf{R}).$$

Here the crystal potential is $V(\mathbf{r}; \mathbf{R})$, the ion coordinates are denoted $\mathbf{R}$, and the self-interactions are contained in the self-energy $S(\mathbf{r}_i; \mathbf{R})$. The band structure $E_n(\mathbf{k})$ can be calculated for this model,

$$\{p^2/2m + V(\mathbf{r}; \mathbf{R}) + S(\mathbf{r}_i; \mathbf{R})\}\psi_{n\mathbf{k}}(\mathbf{r}) = E_n(\mathbf{k})\psi_{n\mathbf{k}}(\mathbf{r}).$$

or, as in the present case, determined by empirically fitting data. Since $S(Sr_i; \mathbf{R})$ is unknown, $E_n(\mathbf{k})$ is not fully specified. Only $e_n(\mathbf{k}) = E_n(\mathbf{k}) - S_{av}$ is determined by the usual bare band structure calculation. Homogeneous deformation of the lattice changes both the crystal potential V and the self-energy S. However, the changes of the average self-energy resulting from deformation can be determined by the requirement that the total energy be a minimum at equilibrium, as demonstrated by Chadi [4].

$$dE_{\text{TOTAL}}/da_L = 0 = \sum_{n\mathbf{k}}{}' de_n(\mathbf{k})/da_L - N dS/da_L,$$

or

$$dS/d\xi = N^{-1} \sum_{n\mathbf{k}}{}' de_n(\mathbf{k})/d\xi \equiv U_1/6.$$

where the primed sums are restricted to the N occupied Bloch states and we have made a crude approximation to the total energy. Thus the deformation potential constant is

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Random superstructures

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Predictions of the densities of states are given for various forms of controlled random disorder in artificial multilayered materials or superstructures.

I. INTRODUCTION

With the development of techniques[1] for fabricating artificial, multilayered, periodic materials, it is possible to study controlled randomness and its effects on electronic states of matter. A hint of the suitability of such superstructured materials for randomness studies was contained in the early work of Esaki and Tsu,[2] but since then the greatest experimental effort has been to remove randomness from superstructures and to make the interfaces between layers abrupt and atomically smooth.

Superstructures with two types of randomness can be grown: randomly varying layer thicknesses and random layer compositions. Both metallic and semiconductor superstructures have been grown, and the ideas of this paper will be applicable to either; however, for definiteness we confine our attention to superstructures composed of layered semiconductors GaAs-$Al_xGa_{1-x}As$, where the random variables are the layer thicknesses d and alloy compositions x. We envision that the stochastic variables d and x are determined by a random number generator during the superstructure growth process and that these quantities are preserved for the analyses of data taken from the superstructured sample.

The resulting disorder is controlled, finite in extent, and essentially one dimensional. Its controlled nature is a valuable aid to understanding random systems, because few such systems have been fabricated before. Moreover, controlled-disorder superlattices offer the possibility of studying heretofore unimagined combinations of order and disorder, such as periodically stacked alternating ordered and disordered arrays. The finiteness of the artificially produced disorder offers opportunities to directly determine the extent of localization of states and to study the impending onset of Anderson localization[3] as a function of increasing size. One dimensional random systems are comparatively well understood theoretically; numerous models have been solved exactly and even more have been thoroughly studied.

For electronic states in semiconductor superstructures three theoretical regimes present themselves: the regime of localized deep-trap-like states,[4] the mixed regime of localized and extended states, and the regime of extended states described by effective-mass theory.[5] The most interesting is the one-band effective-mass theory of carrier motion, which we shall consider. This regime has two subregimes: the quantum well limit[6] in which the effective-mass electron's de Broglie wavelength is comparable with or larger than typical superstructure dimensions, and the classical limit in which the electronic spectrum is characteristic of a classical particle colliding with barriers. In this paper we shall restrict our attention to the quantum well limit.[7,8]

The standard theoretical questions to be answered by any theory of disorder are as follows: (i) What is the ensemble-averaged density of states for the random system? (ii) Are the band gaps of the ordered structure preserved in spite of the disorder or annihilated by it? (iii) Can selected types of disorder *introduce* gaps into a spectrum that would otherwise be continuous? (iv) To what extent does the disorder produce localized states, is diffusion possible, and what is the transmission coefficient for an electron in a random superstructure? (v) What are the effects of "many body" interactions between electrons confined to adjacent layers and can they produce one-dimensional

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HOT ELECTRON DIFFUSION IN FINE LINE SEMICONDUCTOR DEVICES

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Abstract—We present a simple formalism to include hot electron diffusion into device modeling programs. The effectiveness of this method is illustrated for a DMOS-structure and the permeable base transistor. However, the formalism is general and can be applied to any semiconductor device.

1. INTRODUCTION

It is well known that the drift velocity of electrons saturates at high electric fields. This is a consequence of the high carrier energies and increased scattering rates. Stratton[1] derived a simple formalism to include also the changes of the diffusivity D in high electric fields. He showed that if a Maxwellian distribution with a small drift term is assumed, the diffusivity is

$$D = \frac{\mu k T_c}{q} \tag{1}$$

which is formally identical to the Einstein relation. Here μ is the mobility, k is Boltzmann's constant and T_c is the carrier temperature, *not the temperature of the crystal lattice*. Stratton derived (1) with the assumption that the scattering rate depends on the spatial coordinate only through the carrier temperature. His assumptions also exclude anisotropies in the diffusion constant as well as nonlocal effects introduced for example by time dependent friction. These complications will be discussed at the end of the paper where some important references to more exact treatments are given.

The main purpose of the paper is to present a method which maximizes the physical input in the treatment of electronic diffusion in device modelling, while simultaneously minimizing the necessary additional computational effort.

Although the method we present is more general, it is meant for application to silicon devices with dimensions $\geq 0.25 \times 10^{-4}$ cm and for time scales $\geq 5 \times 10^{-12}$ sec.

The key point to note in (1) is that T_c is an increasing function of $\mathbf{F} \cdot \mathbf{j}$ while μ is a decreasing function of $\mathbf{F} \cdot \mathbf{j}$. $\mathbf{F}$ is the electric field and $\mathbf{j}$ is the current density. In many device models the assumption has been made that the carrier temperature, T_c, is equal to the lattice temperature, T_L. This has often given the impression that diffusion currents are unimportant[2–6]. However, for high electric fields and large charge density gradients this assumption causes considerable error in the calculated current densities. Below we demonstrate the effect of properly including the carrier temperature and mobility μ as function of $\mathbf{j} \cdot \mathbf{F}$ and show the significance of this effect for both the diffusion current and the hot electron mobility in devices. The Permeable Base Transistor (PBT) and the Double-Diffused MOS transistor (DMOS) will serve as examples because they exhibit both high electric fields and substantial charge gradients. No attempt was made to precisely determine the diffusion constant. Thus these analyses are qualitative rather than quantitative in nature and the results should not be considered exact. The advantage of our model is that computation time in device modelling programs should not greatly increase when our procedure is used.

2. ANALYTICAL CONSIDERATIONS

Part of the following treatment of high field diffusion in devices has been suggested before for CCD's[7]. We outline the approach here in more detail and emphasize the generality. It is important to notice that the mobility and diffusion constant are not single valued functions of the electric field $\mathbf{F}$. The reason is that the carrier energy, which ultimately determines μ and D, is a function of $\mathbf{j} \cdot \mathbf{F}$, the power input per unit volume as mentioned in the introduction.

For carrier concentrations $n \gg 10^{17}\,\mathrm{cm}^{-3}$ an electron temperature T_c can be defined and the mobility, as well as the diffusion constant, becomes a function of T_c. For $n \ll 10^{17}\,\mathrm{cm}^{-3}$ an electron temperature T_c cannot be defined as the carrier distribution function becomes non-Maxwellian. However, one still can define an average electron energy and the considerations below still apply except for the appearance of statistic factors which leave the treatment qualitatively but not quantitatively valid. Let's assume for the moment that T_c can be defined. The characteristic functional dependence of the mobility on T_c in silicon is then[8]

$$\mu \simeq \mu_0 \sqrt{(T_L/T_c)}. \tag{2}$$

Here, T_L is the temperature of the crystal lattice; eqn (2)

Investigation of Transient Electronic Transport in GaAs Following High Energy Injection

JEFFREY YUH-FONG TANG AND KARL HESS, MEMBER, IEEE

Abstract—We present Monte Carlo simulations of the transient behavior of electrons injected into GaAs at high energies and accelerated (decelerated) by constant electric fields. Our calculations differ from previous calculations due to the inclusion of a realistic band structure (empirical pseudopotential) and the injection of electrons at high energies (e.g., via a heterobarrier). The results show that a narrow "collision-free window" (CFW) exists with respect to parameters such as the external electric field, the injection energy, the external voltages, and the semiconductor dimensions. Within this window average electron velocities of $\sim 8 \times 10^7$ cm/s can be achieved over distances of 10^{-5} cm in emitter (source)- and base-like structures. Voltage (field) parameters typical for the collector (drain) are far outside the CFW and allow only for much reduced (by a factor of ~10) electron velocities. We also discuss thermal noise in "ballistic devices" and show that the noise equivalent temperature can be exceedingly high.

I. Introduction

SINCE THE FIRST calculation of transient electron transport in short-channel FET's by Ruch [1], overshoot phenomena of the electron velocity on very short time and length scales have attracted considerable attention [2]–[5]. Shur [3] and Shur and Eastman [5] added features of space charge limited conditions to the velocity overshoot. They investigated the initial transient and called it the "near ballistic" regime. The term "ballistic" is difficult to define and is currently applied to a wide range of device parameters and dimensions. Investigations in [3] and [5] indicate that "near ballistic" transport over larger distances (>1000 Å), is achievable, necessitates injection of electrons at higher energy. High energy injection was also discussed by Hess [6] for low temperature transport free of scattering events over extremely large distances $L > 10^{-4}$ cm (for electron energies below 0.036 eV).

The criteria for designing devices and choosing materials such that high transient speeds can be advantageously achieved using high energy injection are the key issue of this paper. We approach the problem by a Monte Carlo simulation which includes the details of the band structure as calculated by the empirical pseudopotential method. The electron is started at higher energy values (not at the bottom of the band as done by Ruch) to simulate injection over a (hetero)barrier. The electric field is chosen to be constant over the whole distance of the simulation, in contrast to the choice of the self-consistent field by Shur [3]. The reason for this is the following: Within the CFW, the electron velocity does not vary strongly over the device length because the electrons are already injected at high velocities (in contrast to the cases considered by Shur). Therefore, the carrier concentration is rather constant and the electric field induced by the carriers is of minor importance. In all other respects our calculation is standard. We do not include the intracollisional field effect [7] because it would greatly complicate the computations. In the CFW it also would make only minor contributions since the electric fields in this window are small.

With respect to device applications, the result of the calculations can be summarized as follows: On a length scale of 1000 Å, emitter (source)- and base-like structures may show effects typical for collision-free transport (if carefully designed); collector(drain)-like structures will not.

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II. Physical Model and Method of Computation

As discussed above, we consider high energy electrons injected into GaAs (e.g., from $Al_xGa_{1-x}As$ or δ-like electric fields created by space-charge layers). The transition is assumed to be abrupt, i.e., the electron gains the kinetic energy ΔE and a forward momentum $\Delta \vec{k}$ when transferring to the GaAs without any energy losses.

As illustrated below, the calculations of the self-consistent field resulting from external voltages and electron redistribution in the GaAs is a difficult problem and depends on many details, most importantly:

i) the boundary conditions of the injection,
ii) the statistics of electrons and impurities in the GaAs,
iii) the level of injection, and
iv) the velocity distribution and the injection energy.

Let us assume that our device is short in the x-direction but rather wide in the y-direction. We then can still define average quantities such as the density of electrons in a meaningful way and use a continuum picture as follows: If the distribution function is denoted by f we define electron density

$$n(x) = \frac{2}{(2\pi)^3 L} \int_0^L dy \int_{-\infty}^{+\infty} d\vec{k} f \qquad (1)$$

or the current density as

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ELECTRONIC BAND STRUCTURE OF (001) GaAs–AlAs SUPERLATTICES

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(*Received* 15 *October* 1981 *by F. Bassani*)

We present the results of a theory of electronic energy bands of superlattices using an application of a recent novel empirical tight binding method. The theory is applied to GaAs–AlAs (001) superlattices with very good agreements with available experimental results for both the direct and indirect energy gaps.

SEMICONDUCTOR SUPERLATTICES of alternating layers of GaAs and AlAs have been the subject of extensive investigation [1]. These superlattices provide a means of studying properties of electrons confined to two dimension as well as new materials with properties very much different than their bulk constituents. Some of the experimental results [2] can be explained on the basis of a one dimensional Kronig–Penny model where the AlAs layers are assumed to form potential barriers confining the electrons and holes of GaAs. The barrier heights are obtained from the band edge discontinuity. For a more detailed understanding of the electronic structure of these superlattices, two calculations [3, 4] using empirical pseudopotential (EP) and one calculation [5] using empirical tight-binding (ETB) have been reported. These calculations have been recently discussed [6] and compared to experimental results. The authors [6] noted that only one of these calculations [4] gives results in reasonable agreement with experimental data. In this communication, we present the results of a tight-binding theory for superlattice using an application of a recent novel empirical tight-binding method. Results for the direct and indirect band gaps of a range of monolayer of AlAs and m layers of GaAs superlattices [$(GaAs)_m(AlAs)_1$] for $m = 1, 2, 3$, and 8 are compared to experimental results. The theory provides a good description of the energy gaps over the entire range of these superlattices.

The tight-binding methods as applied to superlattices with alternating layers of GaAs and AlAs have been discussed in detail by Schulman and McGill (SM) [5]. Their methods employ an enlarged unit cell which then describes the superlattice periodicity in the (001) direction. The atoms in each layer are described by tight-binding parameters of the bulk using a Sp^3 basis with nearest and second nearest neighbor interactions. The band edge discontinuity is incorporated by subtracting the valence band discontinuity from the AlAs diagonal bulk parameters. The second nearest neighbor interactions were used to improve the shape of the bulk conduction band.

We have used a method similar to that of SM with some exceptions. We used a recent novel empirical tight-binding method [7] which is able to provide good description of the conduction bands as well as the valence bands of bulk semiconductors by introducing an excited S state into the Sp^3 minimum basis with nearest neighbor interactions. This method provides a convenient and reasonably accurate representation of the bulk band structure for a wide range of semiconductors [7]. As in SM, the valence band edge discontinuity [2] is taken to be 15% of the direct gap differences of GaAs and AlAs and is subtracted from the AlAs diagonal bulk parameters. The resulting matrix of dimension $(n + m) \times 10$ [for $(GaAs)_m(AlAs)_n$ superlattices] is diagonalized numerically to obtain the electronic energy band structure. The available experimental data on the direct and indirect band gaps are very few. To test our theory, we have performed calculations on the series of monolayer superlattices $(GaAs)_m(AlAs)_1$ for which very good experimental results have been explicitly given [8] (for $m = 1, 2, 3$, and 8) including the indirect band gap for the $m = 1$ case. See Fig. 1. Given the theoretical and experimental uncertainty (such as accuracy in description of the bulk band structure, band edge discontinuity and layer thickness fluctuation), the rather good agreement for the $m = 1$ case (both the measured direct and indirect gaps are close to the calculated values) may be fortuitous. The overall agreement over the wide range of $m = 1, 2, 3$, and 8, however, indicates that our theory indeed can provide a good description of the superlattice energy bands within the Slater–Koster [9] interpolating scheme. As was noted in [6], their EP calculations [4] differ from the experimental results by about 60 meV

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Electronic Band Structure of a Model AlP-GaP Superlattice: Indirect to Direct Transition

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Abstract

In this letter we present the first detailed calculation of the electronic band structure of a model (001) AlP-GaP superlattice. The results of the model calculations indicate that a superlattice comprised of indirect AlP and GaP may become a direct semiconductor with a wide band gap ($\sim$ 2.3 ev). Similar transition for other indirect semiconductors are also predicted.

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HIGH ENERGY DIFFUSION EQUATION FOR POLAR SEMICONDUCTORS

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We present a novel method to explicitly solve the Boltzmann equation for highly energetic electrons interacting with polar optical phonons and scattering mainly in forward direction. Our approach reduces the collision integral of the Boltzmann equation into a differential operator which is much easier to manipulate than the integral form and does not require a relaxation time approximation. The spatial diffusion of highly energetic electrons is calculated and discussed in context with high speed velocity transients ("ballistic transport"). Explicit results compare favorably with sophisticated Monte Carlo simulations and are well suited to treat complex transport problems in submicron III-V devices. As an example we calculate the current voltage characteristic of a "camel-back diode".

In polar semiconductors and for highly energetic processes, the scattering of the charge carriers by polar optical phonons (P.O.P.) is mainly in the forward direction, i.e., with conservation of the electron momentum direction. Under these circumstances, the collision integral of the Boltzmann equation is reduced to a differential operator [1,2]

$$C_{P.O.P.} f = \frac{1}{\tau} \left[\hbar\omega \frac{\partial}{\partial \varepsilon} f + \frac{(\hbar\omega)^2}{2\Gamma} \frac{\partial^2}{\partial \varepsilon^2} f \right] \qquad (1)$$

which is much easier to manipulate than the integral form. Here ε is the carrier energy, $1/\tau$ is the spontaneous P.O.P. emission rate, ω is the P.O.P. frequency, and Γ is a factor depending on the temperature T, given by

$$\Gamma = \frac{1 - e^{-z}}{1 + e^{-z}} \qquad (2)$$

with $z = \hbar\omega/k\,T$.

The differential nature of the collision operator, which is of Fokker-Planck type, is well adapted to treat the stochastic processes of non-equilibrium phenomena. Moreover, the solution of the Boltzmann equation does not require the relaxation time approximation, and more general solutions can easily be derived.

A specific application of our theory is the important case (ballistic transport) of steady-state and field-free spatial diffusion of charge injected at high energy. In Fig. 1, the relaxation of an monoenergetic distribution function (D.F.) approximated by a δ-function at the "initial" position $x = 0$ is shown for a parabolic band. Typically, the evolution of the D.F. can be described as follows. Initially, the D.F. is strongly peaked at $\varepsilon = \varepsilon_0$, then

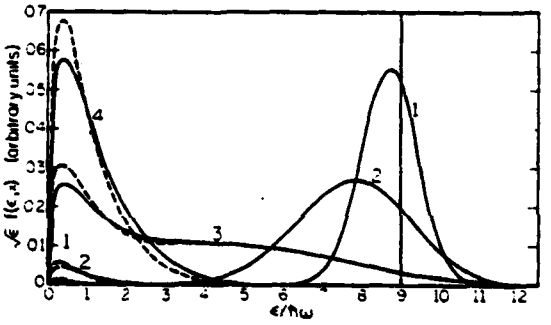

Figure 1: Spatial evolution distribution at T=300K. The starting distribution function (δ-function) is represented by the vertical line at $\varepsilon = \varepsilon_0 = 9\hbar\omega$. 1,2,3, and 4 are for $x\sqrt{\frac{m}{2\varepsilon_0}}/2\Gamma = 0.25, 2, 4$, and ∞ respectively.
Solid line: equilibrium distribution given by Eq. (3)
Dotted line: Maxwell-Boltzmann distribution

under the influence of the P.O.P. scattering, mainly emission, it drifts toward low energy and is broadened. The "drift coefficient" in energy space is given by $\frac{\hbar\omega}{\tau}\sqrt{\frac{m}{2\varepsilon_0}}$ and represents the spontaneous P.O.P. emission. It is independent of the temperature. The broadening factor of the D.F. is proportional to distance and is given by $\frac{2(\hbar\omega)^2 x}{\tau}\sqrt{\frac{m}{2\varepsilon_0}}$. It is an increasing function of the temperature. It is seen that after an infinite distance from the origin, the D.F. reaches its equilibrium profile. From Eq. 1 the equilibrium D.F. is given by

$$C_{P.O.P.} f = 0 \qquad (3)$$

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Energy-diffusion equation for an electron gas interacting with polar optical phonons

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(Received 14 May 1982)

We present a novel method to solve explicitly the Boltzmann equation for highly energetic electrons interacting with polar optical phonons and scattering mainly in the forward direction. In this approach, the collision integral of the Boltzmann equation is reduced to a differential operator which is much easier to manipulate than the integral form and does not require a relaxation-time approximation. The relaxation of the distribution function with time as well as the spatial evolution of highly energetic electrons are calculated and closed-form expressions for the distribution function are given. In both cases the behavior of the electron distribution is characterized by two fundamental parameters: a drift factor which represents the net rate of phonon emission, and a broadening factor which is proportional to the latter and also to time and distance.

I. INTRODUCTION

The theory of high-field transport in semiconductors is closely related to the solution of the Boltzmann equation for high carrier energies.[1] Owing to its complexity (integro-differential equation), the Boltzmann equation cannot be solved explicitly. In the past two general methods of approximation have been proposed. The first relies on the concept of electron temperature and assumes a Maxwellian form of the isotropic part of the electron distribution function.[2,3] Unfortunately, this analytical method applies only to the case of very high electron densities. The other methods use numerical techniques (iterative and Monte Carlo) to solve the Boltzmann equation.[4,5] These methods are more exact but are rather time consuming and costly and therefore not easily applicable to semiconductor device models.

Recently, transient transport phenomena at high energies have been the subject of considerable interest in connection with "ballistic transport" in very short devices.[6] The idea is that for small device dimensions (of the order of the mean free path) the charge carriers suffer only a few collisions and gain extremely high speeds. In the calculations semiempirical (Newton) equations such as the following are often used[7]:

$$\frac{d}{dt}mv_d = qE - \frac{mv_d}{\tau_m}\,, \tag{1a}$$

$$\frac{d}{dt}\epsilon = qv_dE - \frac{\epsilon-\epsilon_0}{\tau_\epsilon}\,, \tag{1b}$$

where ϵ and ϵ_0 are the average and the zero-field energy, respectively, v_d is the drift velocity, E the electric field, m the effective mass, and τ_m and τ_ϵ are the empirical momentum and energy relaxation times.

This method has been subject to controversy since the boundary conditions have been oversimplified and spatial inhomogeneities and the statistical nature of the charge transport have been neglected.[8–10] Moreover, the criteria that define the mean free path are often based on the low-field and steady-state values of the physical parameters, whereas the calculations are applied to high-field and transient phenomena. The numerical methods, Monte Carlo, etc., also have their limitations. In addition to their high cost, they cannot easily be applied to complicated device structures.

In this paper we present a new derivation of the Boltzmann equation for fast electrons scattered by polar optical phonons (POP). This approach can be used to obtain closed-form integrations of the Boltzmann equation even for sophisticated device structures, provided the electrons are injected at high energies and the electric fields away from the injecting barrier can be treated as perturbation. Injection of electrons over barriers was proposed recently[11] to achieve extremely high electron velocities over large distances. It is important in many

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ENERGY DIFFUSION EQUATION FOR AN ELECTRON GAS INTERACTING WITH POLAR OPTICAL PHONONS: NON-PARABOLIC CASE

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(*Received* 19 *August* 1982 *by J. Tauc*)

A novel method previously presented to explicitly solve the Boltzmann equation for highly energetic electrons interacting with polar optical phonons is improved in order to take into account the non-parabolicity of the conduction band. For the case of field free spatial diffusion, the carrier velocity is compared with Monte Carlo simulations. For GaAs the agreement between the analytical and the numerical method is quite good at 77 and 300 K. Also, the results derived for a parabolic band structure show a strong overestimation of the carrier velocity.

IN A PREVIOUS PAPER [1], we presented a novel method to explicitly solve the Boltzmann equation for highly energetic electrons interacting with polar optical phonons (POP). This approach is based on the consideration of forward scattering – i.e., with conservation of the electron momentum direction – due to the electron–POP interaction at high energy. The collision integral of the Boltzmann equation is reduced to a differential operator which is much easier to manipulate than the integral form, and does not require a relaxation time approximation.

In the past similar methods have been applied for both polar [2, 3] and non-polar optical scattering [4, 5]. These phenomenological approaches are restricted to energy space and the distribution function obtained by these methods is only a function of the carrier energy, not of the carrier momentum. Our present method is more general because the differential operator for the POP scattering is directly derived from the Boltzmann equation at high energy. Hence we do not introduce any assumption on the form of the distribution function which contains more information on the transport properties (the streaming effect for example) than a distribution defined in energy space only.

The differential nature of the collision operator, which is similar to a Fokker–Planck equation, is well adapted to treat the stochastic processes of non-equilibrium phenomena [6]. In this respect, this method appears to be a better approximation than previous theories which exclude statistical considerations as well as realistic boundary conditions (ballistic transport theory) [7]. On the other hand, it is less costly than numerical simulations and therefore is easily applicable to semiconductor device models.

The basic derivation has been presented before [1] assuming a parabolic band. The importance of including the nonparabolicity for high energy processes is obvious.

We restrict our considerations to scattering processes in the central Γ-valley and assume that the conduction band is isotropic, omitting any consideration of the satellite valleys. This approximation is reasonable for energies below approximately 0.3 eV in GaAs.

The non-parabolicity of the band is taken into account through the relationship between the electron wavevector $\mathbf{k}$ and its energy ϵ

$$\frac{\hbar^2 k^2}{2m} = \epsilon(1 + \chi\epsilon) \tag{1}$$

where in agreement with Ehrenreich's theory [8]

$$\chi = \frac{1}{\epsilon_g}\left(1 - \frac{m}{m_0}\right) \tag{2}$$

Here ϵ_g is the energy gap and m and m_0 are the effective mass and the free electron mass, respectively. In non-degenerate statistics, the collision integral for electron–POP interaction takes the form

$$\hat{C}_{POP} f = \frac{\alpha}{\pi(1-\gamma)}\frac{(\hbar\omega)^{3/2}}{(2m)^{1/2}}\left[\int \frac{d\mathbf{k}' f(\mathbf{k}')}{|\mathbf{k}-\mathbf{k}'|^2}\{\delta(\epsilon' - \epsilon - \hbar\omega) + \gamma\delta(\epsilon' - \epsilon + \hbar\omega)\} - f(\mathbf{k})\int \frac{d\mathbf{k}'}{|\mathbf{k}-\mathbf{k}'|^2} \times \{\delta(\epsilon' - \epsilon + \hbar\omega) + \gamma\delta(\epsilon' - \epsilon - \hbar\omega)\}\right] \tag{3}$$

where

$$\gamma = \exp\left(-\frac{\hbar\omega}{k_B T}\right).$$

Here α is Fröhlich's electron–phonon coupling constant and ω is the POP frequency [9]. In the forward scattering approximation [1], we obtain

$$\frac{\delta(\epsilon' - \epsilon \mp \hbar\omega)}{|\mathbf{k}' - \mathbf{k}|^2} \cong R_+(\epsilon)\delta(\cos\Theta - 1)\delta(\epsilon' - \epsilon \mp \hbar\omega) \tag{4}$$

Investigation of Transient Electronic Transport in GaAs Following High Energy Injection

JEFFREY YUH-FONG TANG AND KARL HESS, MEMBER, IEEE

Abstract—We present Monte Carlo simulations of the transient behavior of electrons injected into GaAs at high energies and accelerated (decelerated) by constant electric fields. Our calculations differ from previous calculations due to the inclusion of a realistic band structure (empirical pseudopotential) and the injection of electrons at high energies (e.g., via a heterobarrier). The results show that a narrow "collision-free window" (CFW) exists with respect to parameters such as the external electric field, the injection energy, the external voltages, and the semiconductor dimensions. Within this window average electron velocities of $\sim 8 \times 10^7$ cm/s can be achieved over distances of 10^{-5} cm in emitter (source)- and base-like structures. Voltage (field) parameters typical for the collector (drain) are far outside the CFW and allow only for much reduced (by a factor of ~10) electron velocities. We also discuss thermal noise in "ballistic devices" and show that the noise equivalent temperature can be exceedingly high.

I. Introduction

SINCE THE FIRST calculation of transient electron transport in short-channel FET's by Ruch [1], overshoot phenomena of the electron velocity on very short time and length scales have attracted considerable attention [2]–[5]. Shur [3] and Shur and Eastman [5] added features of space charge limited conditions to the velocity overshoot. They investigated the initial transient and called it the "near ballistic" regime. The term "ballistic" is difficult to define and is currently applied to a wide range of device parameters and dimensions. Investigations in [3] and [5] indicate that "near ballistic" transport over larger distances (>1000 Å), is achievable, necessitates injection of electrons at higher energy. High energy injection was also discussed by Hess [6] for low temperature transport free of scattering events over extremely large distances $L \geq 10^{-4}$ cm (for electron energies below 0.036 eV).

The criteria for designing devices and choosing materials such that high transient speeds can be advantageously achieved using high energy injection are the key issue of this paper. We approach the problem by a Monte Carlo simulation which includes the details of the band structure as calculated by the empirical pseudopotential method. The electron is started at higher energy values (not at the bottom of the band as done by Ruch) to simulate injection over a (hetero)barrier. The electric field is chosen to be constant over the whole distance of the simulation, in contrast to the choice of the self-consistent field by Shur [3]. The reason for this is the following: Within the CFW, the electron velocity does not vary strongly over the device length because the electrons are already injected at high velocities (in contrast to the cases considered by Shur). Therefore, the carrier concentration is rather constant and the electric field induced by the carriers is of minor importance. In all other respects our calculation is standard. We do not include the intracollisional field effect [7] because it would greatly complicate the computations. In the CFW it also would make only minor contributions since the electric fields in this window are small.

With respect to device applications, the result of the calculations can be summarized as follows: On a length scale of 1000 Å, emitter (source)- and base-like structures may show effects typical for collision-free transport (if carefully designed); collector(drain)-like structures will not.

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As illustrated below, the calculations of the self-consistent field resulting from external voltages and electron redistribution in the GaAs is a difficult problem and depends on many details, most importantly:

i) the boundary conditions of the injection,
ii) the statistics of electrons and impurities in the GaAs,
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Let us assume that our device is short in the x-direction but rather wide in the y-direction. We then can still define average quantities such as the density of electrons in a meaningful way and use a continuum picture as follows: If the distribution function is denoted by f we define electron density

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or the current density as

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A Jet-Stream Solution for the Current in Planar-Doped-Barrier Devices

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ABSTRACT

An analytical model of hot electron transport over planar-doped-barriers is presented. For long diodes the electronic current is of slow diffusion-like nature ($\leq$ 0.2 μm). For short diodes a "jet-stream solution" for the current has been obtained by solving the Boltzmann transport equation explicitly. Our model is directly applicable to GaAs for barrier heights below the L valleys and confirms the possibility of speed enhancement of such diodes in a limited range of bias-voltage and barrier geometry.

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TRANSIENT TRANSPORT AND TRANSFERRED ELECTRON BEHAVIOR IN GALLIUM ARSENIDE UNDER THE CONDITION OF HIGH-ENERGY ELECTRON INJECTION

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The dynamics of transient transport and transferred electron behavior are studied under the condition of high-energy electron injection. This study makes use of a Monte Carlo simulation with the unique inclusion of realistic band-structure as derived from an empirical pseudopotential method. The Γ-L-X valleys are implicitly coupled, thereby permitting the study of transferred electron behavior in a natural way. The details of the Γ-L-X intervalley electron transfer characteristics are presented showing, for the first time, the dynamical interplay between the X and L valleys. It is readily seen from our results that electron transport in gallium arsenide requires a multivalley description; in addition, the onset of intervalley electron transfer is shown to depend strongly upon the electron injection energy.

Gallium arsenide electronic devices with transit lengths in the submicron and ultrasubmicron regions are coming to fruition due to the advent of MBE[1,2] and MOCVD.[3] The intention of this study is to describe a variety of transient transport characteristics pertinent to gallium arsenide, such as high-speed transport resulting from high-energy electron injection, and the dynamics of transferred electron behavior.

The transport properties described herein are obtained by means of a Monte Carlo simulation. The Monte Carlo method utilized in this paper is unique in that it includes a realistic band-structure as derived from an empirical pseudopotential method. In this simulation, the Γ-L-X valleys are implicitly coupled, thereby permitting the study of transferred electron effects in a natural way.

It is found that the transient velocities achievable in gallium arsenide can be quite large (3-10 X 10^7 cm/sec); however, achievement of such high velocities is shown to depend sensitively upon the electric field, the injection energy, and the transit distance. For devices, as they are currently understood, we show that these speeds can be achieved only in base-(source emitter-) like structures; it is noted that in collector- (drain-) like structures the ever-present high-voltage drops do not permit the manifestation of high-velocity (above saturation-velocity) transport.

Also, we discuss in detail the Γ-X-L intervalley electron transfer characteristics showing, for the first time, the dynamical interplay between the X and L valleys. It is readily seen from our results that electron transport in gallium arsenide generally requires a multivalley description; in addition, the intervalley electron transfer is also shown to be strongly dependent upon the electron injection energy.

The transport properties described herein were obtained by means of a Monte Carlo simulation. The details of the calculations, to within a few minor adjustments, have been discussed elsewhere;[4,5,6] therefore, an in-depth discussion of the simulation is omitted here. In general, the calculation makes use of the following assumptions:

(i) The electrons propagate between scattering events in accordance with the equations of motion

$$\hbar\dot{\vec{k}} = e\vec{E} \qquad (1)$$

and

$$\vec{v} = \frac{1}{\hbar}\nabla_{\vec{k}}\, \varepsilon(\vec{k}) \ . \qquad (2)$$

Here $\vec{E}$, the applied electric field, is constant in space and time, and is assumed to be turned on instantaneously; also, $\varepsilon(\vec{k})$ is the energy-band dispersion relation calculated by the empirical pseudopotential method,[7] but with properly adjusted Γ-L-X intervalley spacings (0.33eV and 0.52eV, respectively).

(ii) Polar optical scattering, acoustic deformation potential scattering, and intervalley scattering mechanisms are taken into account;

Hot Electrons in Semiconductor Heterostructures and Superlattices

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Transient Electronic Transport in InP Under the Condition of High-Energy Electron Injection

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ABSTRACT

Transient transport of electrons in InP is studied under the condition of high-energy electron injection. This study makes use of a Monte Carlo simulation with the unique inclusion of realistic band-structure as derived from an empirical pseudopotential method. The results obtained herein for InP are qualitatively similar to those previously obtained by the authors for GaAs. Quantitatively, it is found that ultrahigh electron drift velocities ($\simeq 10^8$ cm/sec) persist for much higher electric fields and over much longer distance of electron traversal in InP as compared to GaAs.

Monte Carlo Simulation of $n-n^+$ Contact Behavior

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ABSTRACT

We present a Monte Carlo simulation of the behavior of a collecting $n-n^+$ contact in InP. Electrons are injected at high energy into the InP and are accelerated by an applied electric field over a length of ~ 1000 Å. At the collecting contact they encounter a possible reflection back into the device. The reflection coefficient at the contact is chosen to vary between 0 and 0.70. The results show that the average electron drift velocity is greatly lowered at low fields throughout the entire device by the reflection at the contact.

High Field Transport in GaAs, InP, and InAs

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ABSTRACT

Calculations of the steady state and transient electron drift velocities and impact ionization rate are presented for GaAs, InP, and InAs based on a Monte Carlo simulation using a realistic band structure derived from an empirical pseudopotential. The impact ionization results are obtained using collision broadening of the initial state and are found to fit the experimental data well through a wide range of applied fields. In InP the impact ionization rate is much lower than in GaAs and no appreciable anisotropy has been observed. This is due in part to the larger density of states in InP and the corresponding higher electron-phonon scattering rate.

The transient drift velocities are calculated under the condition of high energy injection. The results for InP show that higher velocities can be obtained over 1000 - 1500 Å device lengths for a much larger range of launching energies and applied electric fields than in GaAs. For the case of InAs, due to the large impact ionization rate, high drift velocities can be obtained since the ionization acts to limit the transfer of electrons to the satellite minima. In the absence of impact ionization, the electrons show the usual runaway effect and transfer readily occurs, thus lowering the drift velocity substantially.

Theory of hot electron emission from silicon into silicon dioxide

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We present Monte Carlo simulations of the hot electron emission from silicon into the oxide of metal oxide silicon transistors. The calculations include the pseudopotential band structure and quantum effects such as collision broadening due to the electron–phonon interaction. As a result, we present a set of transport parameters which well describes all hot electron effects in silicon (including saturation velocity and impact ionization). We also show that the collision broadening effect leads to an effective barrier lowering and may require that voltages be scaled down far below the interface barrier height of ~3.1 V in order to avoid hot electron emission.

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I. INTRODUCTION

Electronic transport in the Si/SiO_2 system has been studied extensively because of its important role in silicon device technology. One of the most intriguing problems of hot carrier transport at the Si/SiO_2 interface has been the emission of hot electrons or holes from silicon into SiO_2.[1–4] Various experiments have been performed to study this effect. From our viewpoint, Ning's experimental setup is the most interesting. Ning *et al.*[5,6] measured the absolute emission probability of electrons which were optically generated in the silicon depletion layer and accelerated toward the Si–SiO_2 interface. Past models explaining the emission process involved many simplifying assumptions, for example, an energy independent mean free path and a parabolic band structure. At energies of 3.0 eV above the conduction band edge, the band structure is, of course, highly nonparabolic. Transport at energies at which the emission takes place must also consider different valley types (X,L) and more than one conduction band.[7] Moreover, impact ionization definitely plays an important role.

It is the purpose of this paper to present a Monte Carlo simulation of the hot electron emission process which includes a realistic band structure and quantum effects such as collision broadening. It will be shown that the collision broadening effect introduces an effective barrier lowering which is important for considerations of "scaling away" the hot electron effect.

II. SUMMARY OF EXPERIMENTAL RESULTS

The devices used by Ning *et al.*[5] were n-channel polysilicon–SiO_2–Si field-effect transistors. Electrons are optically generated and injected into SiO_2 as illustrated in Figs. 1(a) and 1(b).[8] Source and drain were grounded, a negative bias was applied to the substrate, and a positive bias was applied to the gate. The advantage of this arrangement is that the gate voltage and the substrate voltage can be varied independently. Optically generated electrons which diffuse into the depletion region are accelerated toward the Si–SiO_2 interface. The majority of carriers that do not overcome the interface barrier are collected and give rise to source and drain currents I_D. The carriers that overcome the barrier contribute to the gate current I_G if they are not trapped in the silicon dioxide layer. By measuring the gate, the source, and the drain currents, the absolute emission probability can be obtained from

$$P=\frac{I_G}{I_{\text{total}}}\simeq\frac{I_G}{2I_D}, \tag{1}$$

where $I_{\text{total}}\sim 2I_D$ is the total current from the substrate.

The doping profile in the silicon substrate can be approximated by a Gaussian distribution

$$N_A(x)=N_B+C_0\exp\left(-\frac{x^2}{2\sigma^2}\right), \tag{2}$$

where x is the distance from the Si–SiO_2 interface, N_B is the

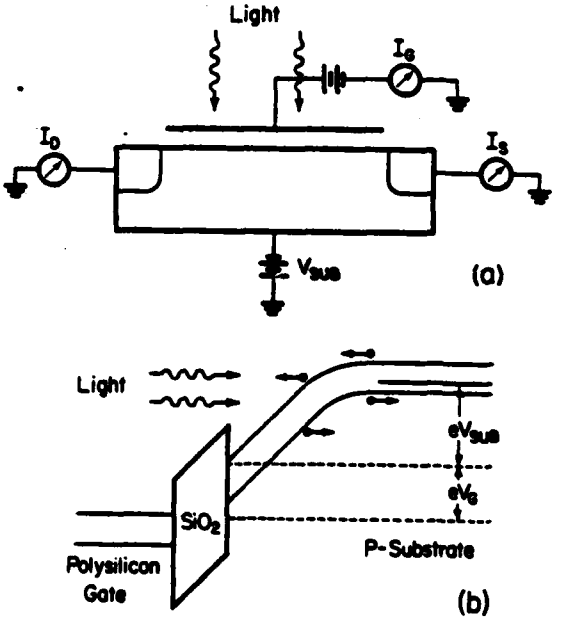

FIG. 1. Experimental arrangement (a) and schematic band-structure diagram (b) defining the hot electron emission from silicon into silicon dioxide.

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Transient Electronic Transport in Staircase Heterostructures

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ABSTRACT

We present a Monte Carlo simulation of electronic transport in new forms of GaAs-GaAlAs heterostructures designed for achieving high drift velocities. Average electron speeds of ~ 5.0×10^7 cm/sec through an entire structure length of 0.5 μm have been calculated. This represents a marked improvement in speed over a single barrier emitter structure. The basic physical principle is the following: the electrons are confined to the gamma valley by losing excess kinetic energy gained from an overlaid accelerating field. The mechanism for the energy loss is a series of ascending potential steps. In this way transfer to the subsidiary minima is avoided and very high velocities are possible. Paradoxically, this means that because the electrons lose kinetic energy their velocity remains high or actually increases.

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scheme. As was noted in [6], their EP calculations [4] differ from the experimental results by about 60 meV